Fthalide 27355-22-2 | DTXSID2058045

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.87	0.81	0.87	0.82	0.86	0.86	

Model Results

Predicted value: 3.83e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.86e-01

Confidence level: 3.50e-01

Nearest Neighbors from the Training Set

Image not found

2,5-Cyclohexadien-1-one, 2,6-dibromo-4-(chloroimino)-

Measured: 1.96e-04 Predicted: 1.41e-03

Image not found

Chloranil

Measured: 1.02e-03 Predicted: 3.29e-03

Image not found

5-methyl-1-phenylpyrrolidin-2-

one

Measured: 1.43e-01 Predicted: 3.13e-01